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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 JAN 17 Pre-1988 INPI data added to MARPAT  
NEWS 4 FEB 21 STN AnaVist, Version 1.1, lets you share your STN AnaVist  
visualization results  
NEWS 5 FEB 22 The IPC thesaurus added to additional patent databases on STN  
NEWS 6 FEB 22 Updates in EPFULL; IPC 8 enhancements added  
NEWS 7 FEB 27 New STN AnaVist pricing effective March 1, 2006  
NEWS 8 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes  
NEWS 9 MAR 22 EMBASE is now updated on a daily basis  
NEWS 10 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL  
NEWS 11 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC  
thesaurus added in PCTFULL  
NEWS 12 APR 04 STN AnaVist \$500 visualization usage credit offered  
NEWS 13 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced  
NEWS 14 APR 12 Improved structure highlighting in FQHIT and QHIT display  
in MARPAT  
NEWS 15 APR 12 Derwent World Patents Index to be reloaded and enhanced during  
second quarter; strategies may be affected  
NEWS 16 MAY 10 CA/CAPLUS enhanced with 1900-1906 U.S. patent records  
NEWS 17 MAY 11 KOREAPAT updates resume  
NEWS 18 MAY 19 Derwent World Patents Index to be reloaded and enhanced  
  
NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.  
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT  
<http://download.cas.org/express/v8.0-Discover/>  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that  
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\* \* \* \* \*

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In an effort to enhance your experience with STN, we would like to better understand what you find useful. Please take approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: <http://www.zoomerang.com/survey.zgi?p=WEB2259HNKWTUW>

Thank you in advance for your participation.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:55:08 ON 24 MAY 2006

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.21             | 0.21          |

FILE 'REGISTRY' ENTERED AT 14:55:20 ON 24 MAY 2006

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

DICTIONARY FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*

\*  
 \* The CA roles and document type information have been removed from \*  
 \* the IDE default display format and the ED field has been added, \*  
 \* effective March 20, 2005. A new display format, IDERL, is now \*  
 \* available and contains the CA role and document type information. \*  
 \*  
 \*\*\*\*\*

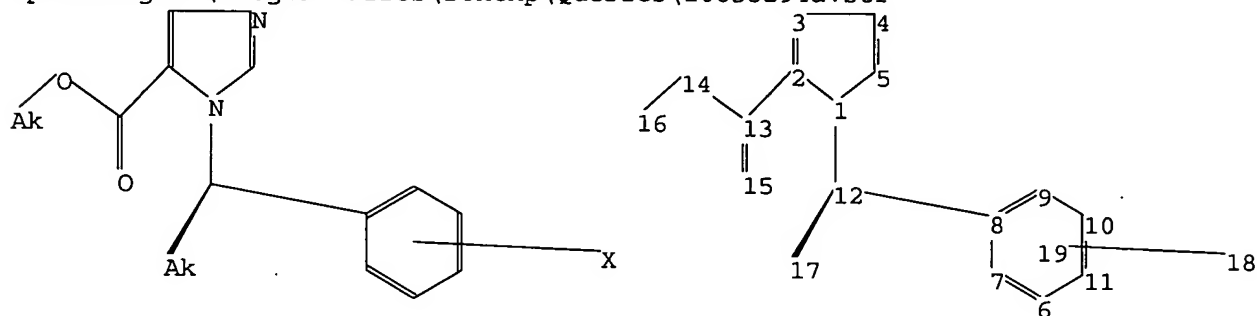
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10635294a.str



chain nodes :  
 12 13 14 15 16 17 18  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 10 11  
 chain bonds :  
 1-12 2-13 8-12 12-17 13-14 13-15 14-16  
 ring bonds :  
 1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11  
 exact/norm bonds :  
 1-2 1-5 1-12 3-4 4-5 12-17 13-14 13-15 14-16  
 exact bonds :  
 2-3 2-13 8-12  
 normalized bonds :  
 6-7 6-11 7-8 8-9 9-10 10-11  
 isolated ring systems :  
 containing 1 : 6 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS

05/24/2006 10635294c.trn

Stereo Bonds:

17-12 (Single Wedge).

Stereo Chiral Centers:

12 (Parity=Don't Care)

Stereo RSS Sets:

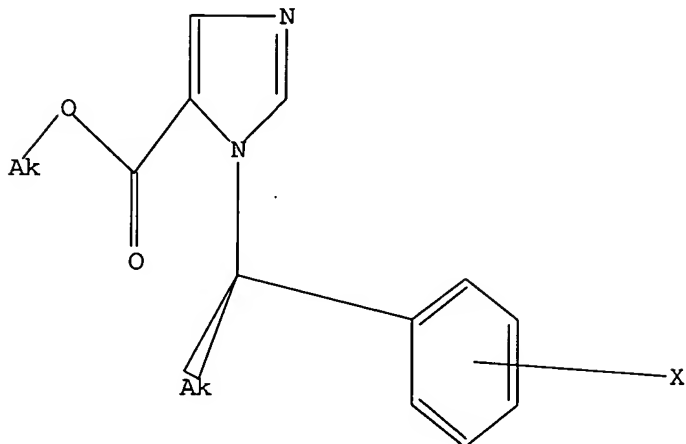
Type=Relative (Default). 1 Nodes= 12

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:55:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 468 TO ITERATE

100.0% PROCESSED 468 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8063 TO 10657

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:55:40 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9425 TO ITERATE

100.0% PROCESSED 9425 ITERATIONS

26 ANSWERS

05/24/2006 10635294c.trn

SEARCH TIME: 00.00.01

L3 26 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'HCAPLUS' ENTERED AT 14:55:46 ON 24 MAY 2006

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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22

FILE LAST UPDATED: 23 May 2006 (20060523/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4

8 L3

=> s 14 and radioactive halogen

173123 RADIOACTIVE

28 RADIOACTIVES

173132 RADIOACTIVE

(RADIOACTIVE OR RADIOACTIVES)

106628 HALOGEN

21560 HALOGENS

117523 HALOGEN

(HALOGEN OR HALOGENS)

78 RADIOACTIVE HALOGEN

(RADIOACTIVE(W) HALOGEN)

L5

1 L4 AND RADIOACTIVE HALOGEN

=> s 14 and radioactive

173123 RADIOACTIVE

28 RADIOACTIVES

173132 RADIOACTIVE

(RADIOACTIVE OR RADIOACTIVES)

L6

2 L4 AND RADIOACTIVE

=> d 15 ibib abs hitstr tot

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:123220 HCAPLUS  
 DOCUMENT NUMBER: 142:198079  
 TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives  
 INVENTOR(S): Zolle, Lise; Hammerschmidt, Friedrich  
 PATENT ASSIGNEE(S): Austria  
 SOURCE: U.S. Pat. Appl. Publ., 15 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO.                        | DATE     |
|------------------------|------|----------|--|----------|
| US 2005033060          | A1   | 20050210 | US 2003-635294                         | 20030806 |
| PRIORITY APPLN. INFO.: |      |          | US 2003-635294                         | 20030806 |
| OTHER SOURCE(S):       |      |          | CASREACT 142:198079; MARPAT 142:198079 |          |
| GI                     |      |          |  |          |

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a **radioactive halogen**] or (II) [X = a nonradioactive or **radioactive halogen** selected from the group consisting of I, Br, and F; X = a **radioactive halogen** selected from the group consisting of 123I, 124I, 131I, 76Br, 82Br or 18F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyl leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2 .5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyl)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX).

IX (30 µg) was reacted with [131I]iodide in 10-20µL 0.05 N aqueous NaOH solution, 15 µL aqueous chloramine-T solution (1 mg/mL), and 6 µL 1 N aqueous HCl

solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[131I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (131I-MTO), i.e. II (R1 = R2 = Me, X = 131I).

IT 813466-09-0P

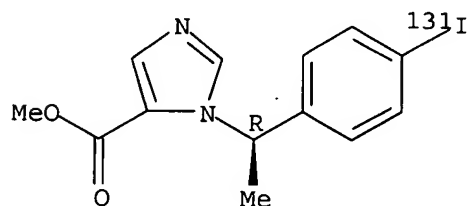
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-09-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 813466-05-6P, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate

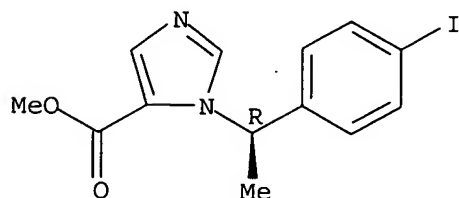
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-05-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



=> d 16 ibib abs hitstr tot

L6 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:123220 HCAPLUS

DOCUMENT NUMBER: 142:198079

TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives

INVENTOR(S): (Zolle, Ilse; Hammerschmidt, Friedrich  
PATENT ASSIGNEE(S): Austria

SOURCE: U.S. Pat. Appl. Publ., 15 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.             | KIND | DATE                                   | APPLICATION NO. | DATE     |
|------------------------|------|--|-----------------|----------|
| US 2005033060          | A1   | 20050210                               | US 2003-635294  | 20030806 |
| PRIORITY APPLN. INFO.: |      |  | US 2003-635294  | 20030806 |
| OTHER SOURCE(S):       |      | CASREACT 142:198079; MARPAT 142:198079 |                 |          |

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a **radioactive** halogen] or (II) [X = a nonradioactive or **radioactive** halogen selected from the group consisting of I, Br, and F; X = a **radioactive** halogen selected from the group consisting of <sup>123</sup>I, <sup>124</sup>I, <sup>131</sup>I, <sup>76</sup>Br, <sup>82</sup>Br or <sup>18</sup>F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-**radioactive** intermediate having trialkylstannyl leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2.5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyl)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX). IX (30 µg) was reacted with [<sup>131</sup>I]iodide in 10-20 µL 0.05 N aqueous NaOH solution, 15 µL aqueous chloramine-T solution (1 mg/mL), and 6 µL 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[<sup>131</sup>I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (<sup>131</sup>I-MTO), i.e. II (R1 = R2 = Me, X = <sup>131</sup>I).



IT 813466-09-0P

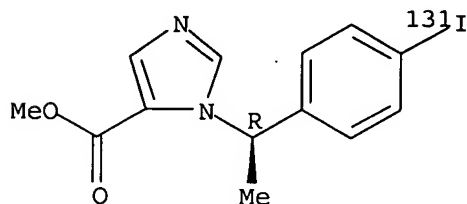
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(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-09-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 813466-05-6P, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate

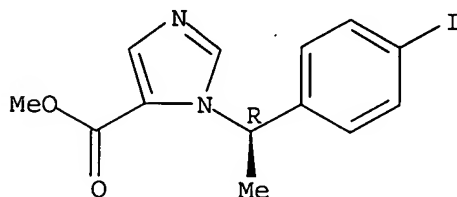
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-05-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L6 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:167377 HCAPLUS

DOCUMENT NUMBER: 108:167377

TITLE: Synthesis of (R)-(+)-3H-etomidate

AUTHOR(S): Janssen, Cor G. M.; Thijssen, Jos B. A.; Verluyten, Willy L. M.; Heykants, Jozef J. P.

CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.

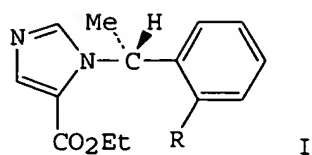
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(8), 909-18  
CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal

LANGUAGE: English

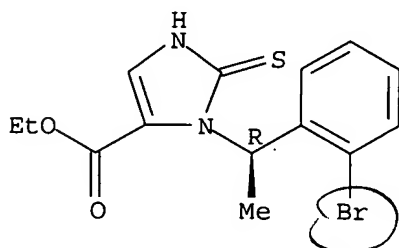
OTHER SOURCE(S): CASREACT 108:167377

GI



- AB Etomideate, (R)-(+)-ethyl-1-(1-phenylethyl)-1H-imidazole-5-carboxylate (I, R = H) is a short-acting hypnotic. A new synthesis, featuring optical resolution of a non-radioactive precursor and introduction of the tritium label by reductive dehalogenation of I (R = Br) is described. I (R = T) was obtained at a specific activity of 3.77 Ci/mmol and a 99.9% purity.
- IT **112366-36-6P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and desulfurization of, with sodium nitrite)
- RN 112366-36-6 HCAPLUS
- CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



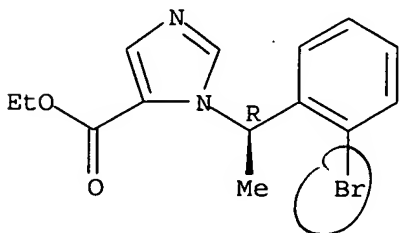
- IT **112366-50-4P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)
- RN 112366-50-4 HCAPLUS
- CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112366-49-1

CMF C14 H15 Br N2 O2

Absolute stereochemistry.

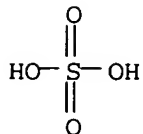


05/24/2006 10635294c.trn

CM 2

CRN 7664-93-9

CMF H2 O4 S



IT 112366-49-1P

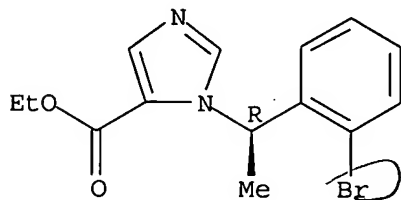
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, reductive debromination, and tritiation of)

RN 112366-49-1 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> log y

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 22.92      | 190.07  |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| -2.25      | -2.25   |

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 14:57:33 ON 24 MAY 2006